



chain nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 17 19 26 31 32 33 34 35 36 37 40
41 42

ring nodes :

24 25 27 28 29 30

chain bonds :

1-2 1-24 2-3 3-4 3-9 3-13 4-5 4-14 4-17 5-6 6-7 7-8 8-40 8-41 8-42 9-10 9-15
10-11 10-12 11-19 19-35 19-36 19-37 25-26 28-31 29-34 30-33 31-32

ring bonds :

24-25 24-27 25-30 27-28 28-29 29-30

exact/norm bonds :

1-24 3-9 4-17 5-6 8-40 8-41 8-42 9-10 9-15 10-12 19-35 19-36 19-37 24-25 24-27
25-26 25-30 27-28 28-29 29-30 29-34 30-33 31-32

exact bonds :

1-2 2-3 3-4 3-13 4-5 4-14 6-7 7-8 10-11 11-19 28-31

G1:CH3,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu,H

G2:OH,MeO,EtO,n-PrO,i-PrO,n-BuO,i-BuO,s-BuO,t-BuO,H

G3:H,O,S,N,P,Si,Cl,Br,F,I

Match level :

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 17:CLASS 19:CLASS 24:Atom 25:Atom
26:CLASS 27:Atom 28:Atom 29:Atom 30:Atom 31:CLASS 32:CLASS 33:CLASS 34:CLASS 35:CLASS
36:CLASS 37:CLASS 40:CLASS 41:CLASS 42:CLASS